

M_F -dependent Hyperfine Induced Transition Rates in an External Magnetic Field for Be-like $^{47}\text{Ti}^{18+}$

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Abstract

Hyperfine induced $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ transition rates in an external magnetic field for Be-like ^{47}Ti were calculated based on the multiconfiguration Dirac-Fock method. It was found that the transition probability is dependent on the magnetic quantum number M_F of the excited state, even in the weak field. The present investigation clarified that the difference of the hyperfine induced transition rate of Be-like Ti ions between experiment [Schippers *et al.*, Phys Rev Lett **98**, (2007) 033001(4)] and theory does not result from the influence of external magnetic field.

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1 Introduction

The hyperfine induced transition (HIT) rate of the $2s2p\ ^3P_0$ level for Be-like ^{47}Ti ions has been measured with high accuracy by means of resonant electron-ion recombination in the heavy-ion storage-ring TSR of the Max-Planck Institute for Nuclear Physics, Heidelberg, Germany [1]. However, the measured transition rate $A_{HIT} = 0.56(3)\ \text{s}^{-1}$ differs from all present theoretical results $A_{HIT} \approx 0.67\ \text{s}^{-1}$ [2, 3, 4] by about 20%. In the theoretical calculations the major part of the electron correlation, which always causes the dominant uncertainty, has been taken into account very elaborately. As a result, it is desirable to find out other reasons for the difference.

In this letter, we focus on the influence of the magnetic field present in the heavy-ion storage-ring on the HIT rate. The HIT rate in an external magnetic field depends on the magnetic quantum number M_F of the excited state, even in a relatively weak field. This effect, combined with the non-statistical distribution of the magnetic sublevel population of the excited level, might lead to the difference in transition rate mentioned above.

2 Theory

In presence of the magnetic field, the Hamiltonian of an atom with non-zero nuclear spin I is

$$H = H_{fs} + H_{hfs} + H_m, \quad (1)$$

where H_{fs} is the relativistic fine-structure Hamiltonian that includes the Breit interaction. H_{hfs} is the hyperfine interaction Hamiltonian, which can be written as a multipole expansion

$$H_{hfs} = \sum_{k \leq 1} \mathbf{T}^{(k)} \cdot \mathbf{M}^{(k)}, \quad (2)$$

where $\mathbf{T}^{(k)}$ and $\mathbf{M}^{(k)}$ are spherical tensor operator in electronic and nuclear space, respectively [5]. H_m is the interaction Hamiltonian with the external homogeneous magnetic field \mathbf{B} ,

$$H_m = (\mathbf{N}^{(1)} + \Delta\mathbf{N}^{(1)}) \cdot \mathbf{B}, \quad (3)$$

where $\mathbf{N}^{(1)}$ are first-order tensor with the similar form of $\mathbf{T}^{(1)}$, $\Delta\mathbf{N}^{(1)}$ is the so called Schwinger QED correction [6].

We choose the direction of the magnetic field as the z -direction, and only M_F is a good quantum number. The wavefunction of the atomic system can thus be written as an expansion

$$|\Upsilon\tilde{\Gamma}IM_F\rangle = \sum_{\Gamma JF} d_{\Gamma JF} |\Upsilon\Gamma IJFM_F\rangle. \quad (4)$$

The total angular momentum \mathbf{F} is coupled by the nuclear \mathbf{I} and electronic \mathbf{J} angular momentum. The Υ and Γ are the other quantum numbers labeling the nuclear and electronic states, respectively.

The coefficients $d_{\Gamma JF}$ in Eq. (4) are obtained through solving the eigenvalue equation using HFSZEEMAN package [7]

$$\mathbf{H}\mathbf{d} = E\mathbf{d}, \quad (5)$$

where \mathbf{H} is the interaction matrix with elements

$$H_{\Gamma JF, \Gamma' J' F'} = \langle \Upsilon\Gamma IJFM_F | H_{fs} + H_{hfs} + H_m | \Upsilon\Gamma' IJ' F' M_F \rangle. \quad (6)$$

The readers are referred to Ref. [6, 7] for a detailed derivation of the different matrix elements.

For the present problem, the wavefunction of the 3P_0 state can be written

$$|“2s2p\ ^3P_0\ I\ M_F”\rangle = d_0 |2s2p\ ^3P_0\ I\ F(=I)\ M_F\rangle + \sum_{S(=1,3); F'} d_{S; F'} |2s2p\ ^SP_1\ I\ F'\ M_F\rangle. \quad (7)$$

The quotation marks in the left-hand wave function emphasize the fact that the notation is just a label indicating the dominant character of the eigenvector. Remaining interactions between $2s2p\ ^3P_0$ and higher members of the Rydberg series can be neglected due to large energy separations and comparatively weak hyperfine couplings [8]. Furthermore, those perturbative states with different total angular momentum \mathbf{F} can be neglected because of relatively weak magnetic interaction. As a result, Eq. (7) is simplified to

$$|“2s2p\ ^3P_0\ I\ M_F”\rangle = d_0 |2s2p\ ^3P_0\ I\ F(=I)\ M_F\rangle + \sum_{S=1,3} d_S |2s2p\ ^SP_1\ I\ F(=I)\ M_F\rangle. \quad (8)$$

Similarly, the wavefunction of the ground state is approximatively written

$$|“2s^2\ ^1S_0\ I\ M_F”\rangle = |2s^2\ ^1S_0\ I\ F(=I)\ M_F\rangle, \quad (9)$$

where all perturbative states were neglected for the same reasons as mentioned above.

The one-photon $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ E1 transition becomes allowed via mixing with the perturbative states of $2s2p\ ^3P_1$ and $2s2p\ ^1P_1$ (see Eq. (8)) induced by both the off-diagonal hyperfine interaction and the interaction with the magnetic field. The decay rate $a(M_F^e)_{HIT}$ from the excited state $|“2s2p\ ^3P_0\ I\ M_F^e”\rangle$ to the ground state $|“2s^2\ ^1S_0\ I\ M_F^g”\rangle$ in s^{-1} is given by

$$a(M_F^e)_{HIT} = \frac{2.02613 \times 10^{18}}{\lambda^3} \sum_q |\langle “2s^2\ ^1S_0\ I\ M_F^g” | P_q^{(1)} | “2s2p\ ^3P_0\ I\ M_F^e” \rangle|^2, \quad (10)$$

Substitute Eq. (8) and (9) into above formula, then

$$a(M_F^e)_{HIT} = \frac{2.02613 \times 10^{18}}{\lambda^3} \sum_q \left| \sum_S d_S \sqrt{2F^g(=I)+1} \sqrt{2F^e(=I)+1} \right. \\ \times \left(\begin{array}{ccc} F^g(=I) & 1 & F^e(=I) \\ -M_{F(=I)}^g & q & M_{F^e(=I)}^e \end{array} \right) \left\{ \begin{array}{ccc} J^g(=0) & F^g(=I) & I \\ F^e(=I) & J^e(=1) & 1 \end{array} \right\} \langle 2s^2\ ^1S_0 || P^{(1)} || 2s2p\ ^S P_1 \rangle|^2. \quad (11)$$

Applying standard tensor algebra, the Eq. (11) is further simplified to

$$a(M_F^e)_{HIT} = \frac{2.02613 \times 10^{18}}{3\lambda^3} (2I+1) \sum_q \left| \sum_S d_S \left(\begin{array}{ccc} I & 1 & I \\ -M_I^g & q & M_I^e \end{array} \right) \langle 2s^2\ ^1S_0 || P^{(1)} || 2s2p\ ^S P_1 \rangle \right|^2, \quad (12)$$

where λ is the wavelength in Å for the transition and $\langle 2s^2\ ^1S_0 || P^{(1)} || 2s2p\ ^S P_1 \rangle$ the reduced electronic transition matrix element in a.u..

From the Eq. (12) we can obtain the Einstein spontaneous emission transition probability [9]

$$A(M_F^e)_{HIT} = \sum_{M_F^g} a(M_F^e)_{HIT} \\ = \frac{2.02613 \times 10^{18}}{3\lambda^3} \left| \sum_S d_S \langle 2s^2\ ^1S_0 || P^{(1)} || 2s2p\ ^S P_1 \rangle \right|^2. \quad (13)$$

It should be noticed that in present approximation of weak magnetic field, i.e., neglecting those perturbative states with different total angular quantum number F , the formula for the transition rate (see Eq. 13) is similar to the one where the transition is induced by only hyperfine interaction [2, 3]. However, a significant difference exists in the mixing coefficients d_S by virtue of incorporating the magnetic interaction into the Hamiltonian for the present work.

The electronic wavefunctions are computed using the GRASP2K program package [10]. Here the wavefunction for a state labeled γJ is approximated by an expansion over jj -coupled configuration state functions (CSFs)

$$|\gamma J\rangle = \sum_i c_i \Phi(\gamma_i J). \quad (14)$$

In the multi-configuration self-consistent field (SCF) procedure both the radial parts of the orbitals and the expansion coefficients c_i are optimized to self-consistency. In the present work a Dirac-Coulomb Hamiltonian is used, and the nucleus is described by an extended Fermi charge distribution [11]. The multi-configuration SCF calculations are followed by relativistic CI calculations including Breit interaction and leading QED effects. In addition, a biorthogonal transformation technique introduced by Malmqvist [12, 13] is used to compute reduced transition matrix elements where the even and odd parity wave functions are built from independently optimized orbital sets.

3 Results and discussion

As a starting point SCF calculations were done for the configurations belonging to the even and odd complex of $n = 2$, respectively. Valence correlation was taken into account by including CSFs obtained by single (S) and double (D) excitations from the even and odd reference configurations to active sets of orbitals. The active sets were systematically increased up to $n \leq 5$. The SCF calculations were followed by CI calculations in which core-valence and core-core correlations and the Breit interaction and QED effects were incorporated. Based on this correlation model, we calculated the hyperfine induced $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ E1 transition rate for Be-like ^{47}Ti ions in absence of the magnetic field to $A_{HIT} = 0.66\text{ s}^{-1}$, where the experimental wavelength 346.99 \AA [14] was used to re-scaled the rate.¹ The value is in good agreement with the other theoretical results: $A_{HIT} = 0.67\text{ s}^{-1}$ by Cheng *et al.* [2] and $A_{HIT} = 0.677\text{ s}^{-1}$ by Andersson *et al.* [3].

Recent theoretical calculations are all in disagreement with the experimental measurement $A = 0.56(3)\text{ s}^{-1}$ [1] by about 20%. It is hypothesized that the discrepancy results from the effect of magnetic field present in the storage ring. Actually, the magnetic field

¹The nucleus of ^{47}Ti has the nuclear spin $I = 5/2$, nuclear dipole moment $\mu = -0.78848$ in μ_N and electric quadrupole moment $Q = 0.3$ in barns [15].

effect has already been noticed and been discussed in previous experiment measuring the lifetime of the hyperfine state of metastable level $5d\ ^4D_{7/2}$ for Xe^+ using the ion storage ring CRYRING at the Manne Siegbahn Laboratory (Stockholm) [16]. Returning to the present problem, experiment was conducted in the heavy-ion storage-ring TSR where the rigidity of the ion beam is given as $B \times \rho = 0.8533\text{ T}$ [1], and the bending radius of the storage ring dipole magnets is $\rho = 1.15\text{m}$ [17]. As a result, the magnetic field in the experiment has been 0.742 T . Considering the factual experimental environment, we calculated the hyperfine induced $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ E1 transition rate of Be-like ^{47}Ti ion in the external magnetic field $B=0.5\text{ T}$, $B=0.742\text{ T}$ and $B=1\text{ T}$, respectively. With assistance of Eq. (12) and Eq. (13), we obtained the transition rate $a(M_F^e)_{\text{HIT}}$ from the excited Zeeman state to the ground Zeeman state, the Einstein transition probability $A(M_F^e)_{\text{HIT}}$ of the excited state, and the corresponding lifetime τ . Computational results are displayed in Table 1. As can be seen from this table, the transition rates $A(M_F^e)_{\text{HIT}}$ for each of the individual excited states “ $2s2p\ ^3P_0 \rightarrow M_F^e$ ” are obviously different because the mixing coefficients d_S in Eq. (13) depend on the magnetic quantum number M_F^e of the excited state.

As can be found from Table 1, the lifetime of 3P_0 level is still not sensitive to the sublevel specific lifetimes, if the magnetic sublevels are populated statistically (the lifetimes $\tau = \sum_{M_F^e} \tau(M_F^e)/(2I + 1) = 1.52\text{s}, 1.52\text{s}, 1.53\text{s}$ in the external magnetic field $B=0.5\text{T}$, 0.742T and 1T , respectively). In this case, the zero-field lifetime within the exponential error can be obtained, as made in Ref. [1], through only a fit of one exponential decay curve instead of 6 exponential decay curves with slightly different decay constants. To the contrary, in the experiment measuring the HIT rate of the $2s2p\ ^3P_0$ level of the Be-like Ti ion, the level concerned was produced through beam-foil excitation [18]. As we know, the cross sections with magnetic sublevels for ion-atom collision are different [19, 20], and the magnetic sublevel population is in general not statistically distributed. Combining this fact with the M_F -dependent HIT rate in an external field, the transition probability of 3P_0 level cannot be obtained by statistical average over all magnetic sublevel. However, we also noticed that an external magnetic field can lower the transition rate only for those magnetic sublevels with $M_F \geq 0$. In other word, only if these specific magnetic sublevels with $M_F \geq 0$ were populated, it is possible to explain or decrease the discrepancy between the measured and theoretical HIT rates for Be-like ^{47}Ti . In fact, such extreme orientation of the stored ions seems improbable by means of beam-foil excitation. Moreover, the experimental

heavy-ion storage-ring was only partly covered with dipole magnets (this fraction amounts to 13%) [17]. It further reduces the influence of magnetic field on the lifetime of level. Therefore, we still cannot clarify the disagreement between experimental measurement and theoretical calculations at present even though the influence of an external magnetic field was taken into account.

4 Summary

To sum up, we have calculated the hyperfine induced $2s2s\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ E1 transition rate in an external magnetic field for each of the magnetic sub-hyperfine levels of $^{47}\text{Ti}^{18+}$ ions based on the multiconfiguration Dirac-Fock method. It was found that the transition rate is dependent on the magnetic quantum number M_F^e of the excited state, even in relatively weak magnetic fields. Considering the influence of an external magnetic field, we still did not explain the difference in the HIT rate of Be-like Ti ion between experiment and theory.

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Table 1: Hyperfine induced $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ E1 transition rates in presence of magnetic field B=0.5 T, B=0.742 T and B=1 T for Be-like ^{47}Ti ion. a represents the transition probability from the excited state “ $2s2p\ ^3P_0\ I\ M_F^e$ ” to the ground state “ $2s^2\ ^1S_0\ I\ M_F^g$ ”, A is the Einstein transition probability from the excited state “ $2s2p\ ^3P_0\ I\ M_F^e$ ”. τ is the lifetime of excited state “ $2s2p\ ^3P_0\ I\ M_F^e$ ”. The experimental wavelength (λ) 346.99 Å[14] was used in this calculations, where the influence of hyperfine interaction and magnetic field was neglected.

M_F^e	M_F^g	ΔM	B=0.5 T			B=0.742 T			B=1 T		
			$a\ (\text{s}^{-1})$	$A\ (\text{s}^{-1})$	$\tau\ (\text{s})$	$a\ (\text{s}^{-1})$	$A\ (\text{s}^{-1})$	$\tau\ (\text{s})$	$a\ (\text{s}^{-1})$	$A\ (\text{s}^{-1})$	$\tau\ (\text{s})$
5/2	5/2	0	0.44	0.61	1.64	0.42	0.59	1.71	0.40	0.56	1.78
	3/2	-1	0.17			0.17			0.16		
3/2	5/2	1	0.18	0.63	1.59	0.18	0.62	1.62	0.17	0.60	1.67
	3/2	0	0.16			0.16			0.15		
	1/2	-1	0.29			0.28			0.27		
1/2	3/2	1	0.30	0.65	1.54	0.30	0.65	1.55	0.29	0.64	1.56
	1/2	0	0.02			0.02			0.02		
	-1/2	-1	0.33			0.33			0.33		
-1/2	1/2	1	0.35	0.67	1.49	0.35	0.68	1.48	0.35	0.68	1.47
	-1/2	0	0.02			0.02			0.02		
	-3/2	-1	0.31			0.31			0.31		
-3/2	-1/2	1	0.32	0.69	1.44	0.32	0.71	1.41	0.33	0.73	1.38
	-3/2	0	0.18			0.18			0.19		
	-5/2	-1	0.20			0.20			0.21		
-5/2	-3/2	1	0.20	0.71	1.40	0.21	0.74	1.35	0.22	0.77	1.30
	-5/2	0	0.51			0.53			0.55		